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COMPUTATIONAL INVESTIGATION OF THE STABILITIES OF SOME PROPOSED MOLECULES AND MOLECULAR-ANIONS

by

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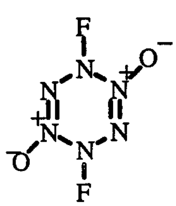
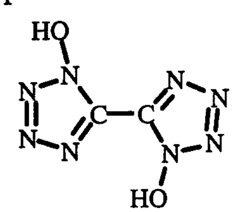
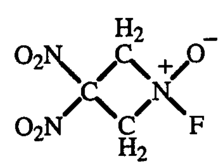
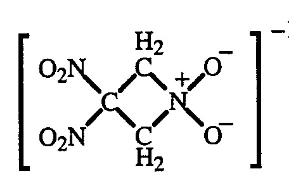
13. ABSTRACT (Maximum 200 words)

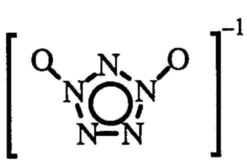
Density functional computational studies have shown that **1 - 6** do correspond to energy minima. Their calculated bond lengths are presented and discussed.

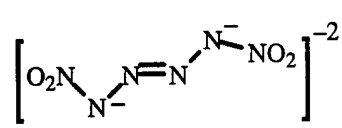
1 

2 

3 

4 

5 

6 

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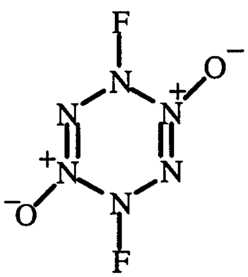
We have investigated the thermodynamic stabilities of the molecules and molecular-anions **1 - 6**. These have been suggested by R. Schmitt and J. Bottaro (SRI) as potential energetic systems. Our procedure in each case is to compute the optimized geometry and the associated vibration frequencies; if none of the latter are found to be imaginary, then the structure corresponds to an energy minimum [1].



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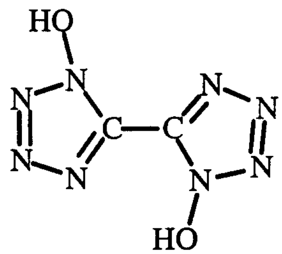

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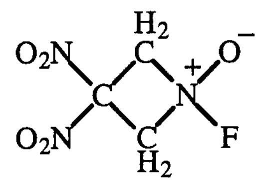

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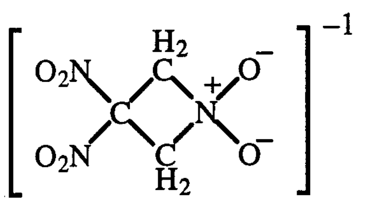

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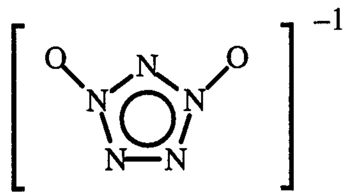

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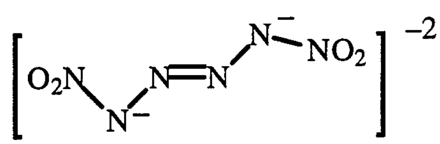

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The B3P86 density functional computational procedure was used [2]; the basis sets were 6-31G* for **3**, 6–31G** for **1**, **4** and **5**, and 6-31+G** for **2** and **6**. None of the systems **1 – 6** were found to have any imaginary vibration frequencies. This confirms that their optimized geometries do correspond to energy minima and that these molecules and molecular-ions should in principle be able to exist.

The computed bond lengths in **1 – 6** are shown in Figure 1. Some points to note are:

(1) The unusually long N–N bonds in **1** (1.538 and 1.550 Å). These are more than 0.1 Å longer than is normal for analogous circumstances [3].

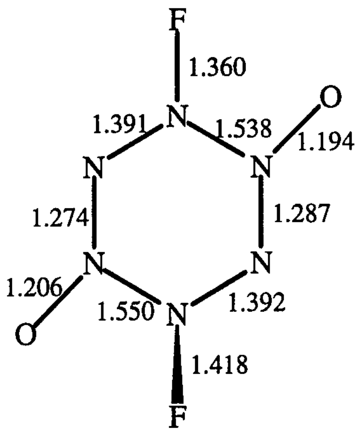
(2) The similarity of the ring bond lengths in **2**.

(3) The very long N–F bond in **3**.

(4) The contrasting N^+–O^- distances in **1**, **3**, **4** and **5**. For comparison, the N^+–O^- bond length is 1.234 Å in furoxan and 1.304 Å in pyridine N-oxide [3].

References:

1. W. J. Hehre, L. Radom, P. v. R. Schleyer and J. A. Pople, *Ab Initio Molecular Orbital Theory*, Wiley-Interscience, New York, 1986 .
2. M. J. Frisch, G. W. Trucks, H. B. Schlegel, P. M. W. Gill, B. G. Johnson, M. A. Robb, J. R. Cheeseman, T. A. Keith, G. A. Petersson, J. A. Montgomery, K. Raghavachari, M. A. Al-Laham, V. G. Zakrezewski, J. V. Ortiz, J. B. Foresman, J. Cioslowski, B. B. Stefanov, A. Nanayakkara, M. Challacombe, C. Y. Peng, P. Y. Ayala, W. Chen, M. W. Wong, J. L. Andres, E. S. Replogle, R. Gomperts, R. L. Martin, D. J. Fox, J. S. Binkley, D. J. Defrees, J. Baker, J. P. Stewart, M. Head-Gordon, C. Gonzalez and J. A. Pople, Gaussian 94, (Gaussian, Inc., Pittsburgh, PA, 1995).
3. F. H. Allen, O. Kennard, D. G. Watson, L. Brammer, A. G. Orpen and R. Taylor, J. Chem. Soc. Perkin II , S1 (1987).



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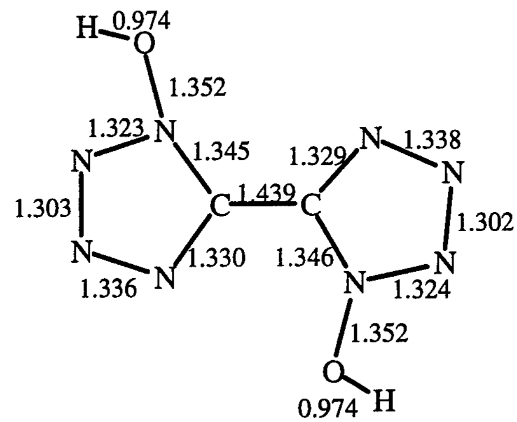
(ring has boat conformation)



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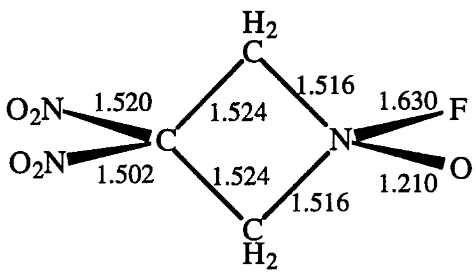
(the rings are within 8° of coplanarity)



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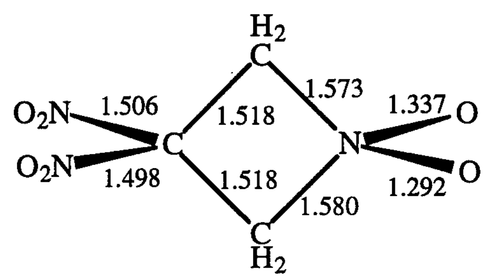

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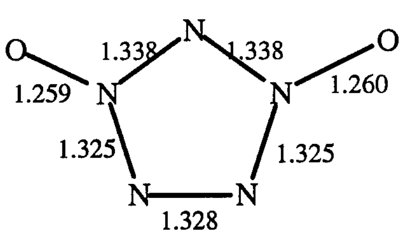

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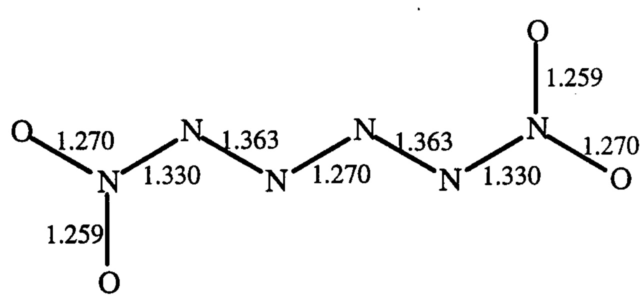

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Figure 1. Computed bond lengths.